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THE ROLE OF SOMMERVILLE TETRAHEDRA IN NUMERICAL MATHEMATICS

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Abstract: In this paper we summarize three recent results in computational geometry, that were motivated by applications in mathematical modelling of fluids. The cornerstone of all three results is the genuine construction developed by D. Sommerville already in 1923. We show *Sommerville tetrahedra* can be effectively used as an underlying mesh with additional properties and also can help us prove a result on boundary-fitted meshes. Finally we demonstrate the universality of the Sommerville's construction by its direct generalization to any dimension.

Keywords: simplicial tessellations, simplicial mesh, Sommerville tetrahedron, well-centered mesh, boundary-fitted mesh, high dimension

MSC: 51M20, 51M04, 65N30, 65N50.

1. Introduction

Many computational methods require or prefer simplicial meshes as the underlying geometrical playground. In two dimensions the best triangle among all, measured by various regularity criteria, is the equilateral triangle, which is a space-filler. In higher dimensions the situation is different, as already for $d = 3$ the equilateral tetrahedron cannot tile the space, see [13].

If the equilateral tetrahedron cannot be taken as the standard, is there any other playing such role what concerns space-filling? The answer is affirmative, as we show in the sequel. Moreover, an answer to that question will be generalized to a general dimension.

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The cornerstone of this paper is the construction proposed by Sommerville already in 1923, see [14]. It takes the unit equilateral triangle $A_0A_1A_2$ as a base and creates the points $B_0, B_1, B_2, \ldots$ above the three original points satisfying

$$B_z = [A_{i(z)}, zp], z \in \mathbb{Z}, \qquad \text{where} \quad i(z) \equiv z \mod 3, \tag{1}$$

and p is a positive parameter. Then the tetrahedra are defined as convex hulls of four consecutive points, which we denote $\mathrm{co}\{B_z, B_{z+1}, B_{z+2}, B_{z+3}\} =: K_3^z$. Three such tetrahedra are sketched in Figure 1. Obviously, this construction enables to fill the whole infinite triangular prism by copies of a single element. Repeating this construction appropriately above all triangles, one gets a face-to-face tessellation of the three-dimensional space, determined up to a positive constant p, that consists of congruent tetrahedra, whose representative is denoted by $K_3(p)$. For more details we refer to [7].

The paper is devoted to three recent author's results based on the above construction. These can be found in their full detail in [7], [9] and [8]; here we provide their brief summary with some additional comments. Each of these results is presented in a separate section.

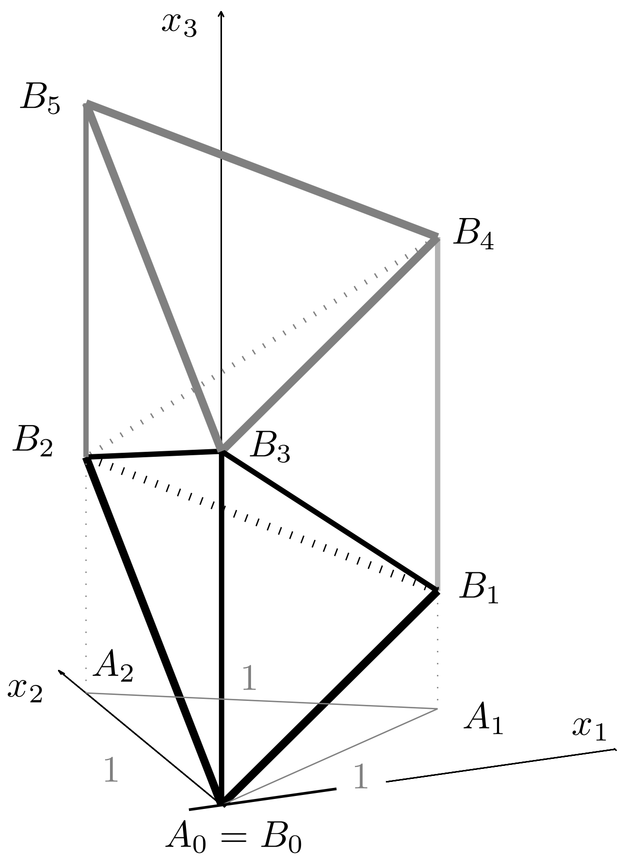

Figure 1: Illustration of the Sommerville's construction.

2. Well-centered Sommerville tetrahedra and their shape-optimization

This result was motivated by the work of Feireisl et al. [4], in which the convergence of a numerical scheme to the compressible Navier-Stokes-Fourier system in three spatial dimensions is proven. While the target system is confined to a smooth bounded domain Ω, the numerical scheme is supposed to be defined on a family of polyhedral domains $\{\Omega_h\}_{h\to 0}$, for which $\Omega \subset \Omega_h$ and $\max_{x\in\partial\Omega_h} \operatorname{dist}[x, \partial\Omega] \le h$. This approach, known as *variational crime*, see e.g. [2], is known to decrease the rate of convergence, upon the condition that conforming elements are used. This is, however, not the case in [4], where non-conforming Crouzeix-Raviart elements are used for velocity.

Numerical domains Ω_h are supposed to admit face-to-face tetrahedral meshes $\mathcal{T}_h$ (where h denotes the characteristic diameter of the elements), satisfying the strong regularity property.

Definition 1 (Strong regularity)**.** Let $\{\mathcal{T}_h\}_{h\to 0}$ be a family of meshes. If there exists $\theta_0 > 0$ independent of h such that for any $\mathcal{T}_h$ and any $K \in \mathcal{T}_h$ it holds that

$$\theta(K) := \frac{\varrho(K)}{\operatorname{diam} K} \ge \theta_0, \tag{2}$$

where $\varrho(K)$ is the radius of the largest ball contained in K, then we say that $\{\mathcal{T}_h\}_{h\to 0}$ is a *strongly regular* family.

One can also define strong regularity with different regularity ratios. Equivalency of some of these definitions can be found in [1]. The terms *shape regular* or *regular* family of meshes can be found within the literature for the property (2).

Further, the tetrahedral elements of the mesh in [4] is assumed to satisfy so-called *well-centered property*, introduced by VanderZee, see e.g. [16]. A well-centered simplex contains its circumcenter in its interior; this ensures that the segment connecting the circumcenters of two neighbouring elements is perpendicular to their common facet and does not degenerate. This property is used in the numerical scheme for the balance of temperature. For the sake of brevity, we use the term *well-centered* mesh instead of the more proper *d-well-centered* mesh.

Definition 2 (Well-centered property)**.** Let $K_d := \operatorname{co}\{V_0, V_1, \dots, V_d\}$ be an d-dimensional simplex. We say that K_d is well-centered if its circumcenter lies in the interior of K_d.

We would like to point out that in two dimensions the well-centeredness coincides with acuteness, while in higher dimensions it is no longer true, see some illustrations in [15].

With all the above said, the idea for finding the polyhedral domains Ω_h and meshes $\mathcal{T}_h$ was the following. First, to find a face-to-face well-centered tetrahedral tessellation of the whole three-dimensional space with the size of the elements not exceeding h and then to pick those elements whose intersection with Ω is non-empty. Their union then builds Ω_h.

We use the Sommerville's result, which can be scaled to provide the desired tessellation. By virtue of a sufficient condition introduced by VanderZee, [16, Theorem 1] and elementary geometric calculations, we are able to determine the range of parameters, for which the elements are well-centered.

Theorem 1 ([7], Theorem 3.3)**.** *The tetrahedra constructed by the method described in Section 1 are well-centered if and only if* $p \in \big(0, \sqrt{2}/2\big)$.

Basically any parameter from given range would give a satisfactory mesh. However, it is obvious that parameters in the middle of the interval are *better* than those at its edges; for p small we obtain flat tetrahedra of the *wedge* type that are close to degenerate ones, while for $p \to \sqrt{2}/2$ the distances of neighbouring circumcenters degenerate. Therefore, we determine a *shape optimal parameter* within this range.

Theorem 2. *Let* $K_3(p)$ *be a tetrahedron constructed by the method in Section 1 and let* θ *be the regularity ratio defined by (2). Then* $\theta(p) := \theta(K_3(p))$ *is maximal for* $p = p^\star = \sqrt{2}/4$.

The value $p^\star$ is optimal also for regularity ratio (6) that is used later in Section 4 and also for the ratio of circumradius and inradius of an element, which is the original assertion [7, Theorem 4.3].

While the general $p \in (0, \sqrt{2}/2)$ gives a well-centered mesh that consists of a tetrahedra that are congruent to each other, for $p^\star$ we get a mesh build by copies of a single element, which also trivially implies the strong regularity property. The element is an *equifacial tetrahedron*, see [6]. As for Naylor [12], it is the most regular tetrahedron, whose copies tile the three dimensional space. Thus it can (and in the next section will) be used as a reference tetrahedron for measuring the shape regularity.

3. Strongly regular family of boundary-fitted meshes

The second result is also motivated by a numerical scheme for compressible flow on an unfitted mesh. For establishing error estimates to a numerical scheme for compressible Navier-Stokes equation in three dimensions in [3], the weak-strong uniqueness principle, see [5], is used. For this reason, the existence of a strong solution is assumed. But the system is known to possess strong solution only on sufficiently smooth domains. Therefore, the target system is confined to a bounded domain $\Omega \in C^3$, while the numerical scheme is designed on a tetrahedral mesh $\mathcal{T}_h$ that fills a polyhedral domain Ω_h. There is no inclusion of the domains Ω_h and Ω assumed, but both domains shall be close to each other. We require for all $x \in \partial\Omega_h$ that

$$\mathrm{dist}[x, \partial\Omega] \leq d_\Omega h^2, \tag{3}$$

with the constant d_Ω depending solely on the geometry of Ω. This is easily ensured by placing the vertices of the polyhedral domain Ω_h at the boundary of the smooth domain Ω. We call such mesh *boundary-fitted*. To prove (3), one just uses the Taylor expansion.

Again, for the convergence, we need to assume that the family of polyhedral domains is strongly regular. The question of existence of a strongly regular family of boundary-fitted simplicial meshes to a C^2 domain is affirmative in two dimensions thanks to [10]. We attack the three-dimensional case and the result reads as follows.

Theorem 3 ([9], Theorem 1)**.** *Let Ω be a bounded domain in $\mathbb{R}^3$ of the class C^2, with the minimal radius of an osculation sphere equal to r_Ω. Let for some h_1* sufficiently small *there exists $(\Omega_{h_1}, \mathcal{T}_{h_1})$ an approximative domain with boundary-fitted mesh and let*

$$\theta(K) \geq \frac{\alpha}{r_\Omega} \text{diam } K,$$

for any $K \in \mathcal{T}_{h_1}$, where θ is defined in (2) and $\alpha > \alpha_0 = 32(2+\sqrt{5})\sqrt{2/3}$.

Then there exists a strongly regular family of boundary-fitted meshes $\{\mathcal{T}_h\}_{h\to 0}$.

The assumption is easy to be fulfilled, as the initial regularity requirement gets weaker with decreasing discretization parameter. The proof is based on the result of Křížek, see [11], that shows that a Sommerville tetrahedron, i.e. tetrahedron $K_3(p^\star)$ from Section 2, can be decomposed into eight identical tetrahedra that are similar to the original one. As a consequence, any tetrahedron of the size h can be decomposed into eight tetrahedra of the size not exceeding $h/2$ while the regularity is preserved. Hence we decompose the initial mesh, the newly established vertices that lie on $\partial\Omega_h$ get shifted to the smooth boundary $\partial\Omega$ and we show, that the regularity does not deteriorate *too much*. The shifts of these vertices are performed by affine mappings. This was our motivation to employ a new regularity criterion, based on the similarity of a tetrahedron with the reference one, Sommerville tetrahedron.

Definition 3. Let $K = \text{co}\{A, B, C, D\}$ be a tetrahedron,

$$\mathcal{A}_K := \{F_K; F_K \text{ an affine transformation}, F_K(\widetilde{K}) = K\}$$

be a set of all affine transformations mapping Sommerville tetrahedron $\widetilde{K}$ onto K. Then we define the *Sommerville regularity ratio* of tetrahedron K as

$$\kappa(K) = \max_{F_K \in \mathcal{A}_K} \frac{\sigma_{\min}(F_K)}{\sigma_{\max}(F_K)},$$

where $\sigma_{\min}(F_K), \sigma_{\max}(F_K)$ are the minimal and maximal singular values of F_K.

We are able to show, that this regularity criterion is equivalent to the other standard ones in the sense of strong regularity, hence the whole proof can be performed in the terms of κ. The details of the laborious and technical proof can be found in [9]. Here we just point out that the final argument is based on the following inequalities,

$$\prod_{j=0}^{n-1}(1 - aq^j) > \lim_{n\to\infty} \prod_{j=0}^{n-1}(1 - aq^j) = P(a, q) > 0,$$

for any $n \in \mathbb{N}$ and $a, q \in [0, 1]$.

4. Space-filling simplices in general dimension

The last of the triplet of results is motivated by the Sommerville's construction itself. One can view it as a method of creating the tessellation of d-dimensional space out of $(d-1)$-dimensional one.

The idea is to take a simplex of a tessellation of the $(d-1)$-dimensional space and create the infinite prism made of d-dimensional simplices above it. More specifically, for a simplex $K \in \mathcal{T}_{d-1}$, where $K = \mathrm{co}\{A_0, A_1, \ldots, A_{d-1}\}$ we construct points B_z satisfying

$$B_z = [A_{i(z)}, zp], z \in \mathbb{Z}, \qquad \text{where} \quad i(z) \equiv z \mod d, \tag{4}$$

compare (4) with (1). The simplices are defined as convex hulls of $d+1$ consecutive points B_z. Performing the same above all simplices of the original $(d-1)$-dimensional tessellation, one recovers a face-to-face simplicial tessellation of d-dimensional space, as it is summarized in the following lemma.

Lemma 1 ([8], Lemma 2.2)**.** *Let $d \geq 2$ and $\mathcal{T}_{d-1} = \{K^k_{d-1}\}_{k\in\mathbb{Z}^{d-1}}$ be a simplicial tessellation of $(d-1)$-dimensional space such that the graph constructed from vertices and edges of $\mathcal{T}_{d-1}$ is a d-vertex-colorable graph. Then*

- *there exists $\mathcal{T}_d = \{L^l_d\}_{l\in\mathbb{Z}^d}$ a simplicial tessellation of d-dimensional space with additional shape parameter p_d,*
- *any connected compact subset of $\mathcal{T}_d$ is a face-to-face mesh,*
- *$\mathcal{T}_d$ is a $(d+1)$-vertex-colorable graph.*

The vertex coloring is a tool which ensures the face-to-face property and guarantees that above a vertex (that is shared by several simplices) the new points are constructed consistently, in the same heights above each element. Lemma 1 provides us with the induction step, the initial step is given as a straight line discretized equidistantly using $p_1 > 0$ with points of alternating colors. Thus, we can state the following.

Theorem 4 ([8], Theorem 2.1)**.** *For any d-dimensional space there exists a d-parametric family of simplicial tessellations $\mathcal{T}_d(\mathbf{p}), \mathbf{p} = (p_1, p_2, \ldots, p_d), p_i > 0$. For $\mathbf{p}$ fixed, all elements $K \in \mathcal{T}_d(\mathbf{p})$ have the same d-dimensional measure equal to*

$$\mathrm{meas}_d K = \prod_{i=1}^{d} p_i. \tag{5}$$

Moreover, every connected compact subset of the tessellation builds a face-to-face mesh.

We obtained a tessellation that is determined up to a d-dimensional vector of positive parameters $\mathbf{p} = (p_1, \ldots, p_d)$. Therefore, we determine the shape-optimal vector of parameters. To benefit from the equivolumetricity property (5), we decided to optimize the ratio

$$\vartheta(K) = \frac{\text{meas}_d K}{(\text{diam } K)^d}, \qquad d \geq 2. \tag{6}$$

In particular, we are looking for an element $K^\star$ and a vector $\mathbf{p}^\star$ satisfying

$$\vartheta(K^\star(\mathbf{p}^\star)) = \sup_{\mathbf{p}\in\mathbb{R}^d_+} \min_{K\in\mathcal{T}_d(\mathbf{p})} \frac{\text{meas}_d K}{(\text{diam } K)^d}, \tag{7}$$

as in general all the elements are not equal. We are optimizing the *worst* element, which is the one with largest diameter. Luckily, there is only a limited number of candidates for the diameter, therefore (7) can be viewed as an optimization problem with nonlinear constraints. Such optimum must satisfy so-called Karush-Kuhn-Tucker conditions. These are always necessary, but sufficient only when the optimized function is convex.

Since we are not able to show the convexity, we prove that the minimizer exists and that there is a unique vector $\mathbf{p}^\star$ that satisfies these conditions. Then $\mathbf{p}^\star$ must be the minimizer. To be precise, the above is true after fixing p_1, which obviously plays the role of a scaling parameter and as such does not affect the shape of the simplices. The statement reads as follows.

Theorem 5 ([8], Theorem 3.1)**.** *Let $d \geq 2$ and let $\mathcal{T}_d(\mathbf{p})$ be a tessellation constructed through the procedure introduced above. Then there exists a unique one-dimensional vector half-space*

$$P^\star = \left\{ \mathbf{p}^{\star,\kappa} \in \mathbb{R}^d_+ | \mathbf{p}^{\star,\kappa} = \kappa\mathbf{p}^\star, \kappa > 0, p_1^\star = 1, p_2^\star = \frac{1}{\sqrt{3}}, p_j^\star = \frac{1}{j-1}\sqrt{\frac{2}{3}}, j \in \{3,\ldots,d\} \right\},$$

of optimal parameters that realize

$$\sup_{\mathbf{p}\in\mathbb{R}^d_+} \min_{K\in\mathcal{T}_d(\mathbf{p})} \frac{\text{meas}_d K}{(\text{diam } K)^d}. \tag{8}$$

The detailed proof can be found in [8]. Here we just point out two interesting remarks.

The result of the optimization would be the same, if one optimizes at every level of the construction, which is a one-dimensional optimization that is much easier. In other words, a shape optimal tessellation cannot be created from a sub-optimal tessellation of a hyperplane.

As it was already mentioned in Section 2, for $d = 3$ we obtain again the (equifacial) Sommerville tetrahedron. One can verify that for the choice $\kappa = \sqrt{3}/2$ we get unit equilateral triangle for $d = 2$, which was the base for construction in Section 2, indeed $\kappa p_3^\star = \sqrt{2}/4$.

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